

## Dynamics of solid proteins by means of Nuclear Magnetic Resonance Relaxometry

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Fast Field-Cycling relaxometry is an NMR technique used to determine the spin-lattice relaxation rates ( $R_1$ ) of samples as a function of resonant frequency (or, equivalently, magnetic field strength). When studied over wide range of frequencies,  $R_1(\omega)$  (the relaxation dispersion profile) provides information on molecular dynamics of the system under investigation.

Due to the presence of  $^{14}\text{N}$  nuclei in the structure of amide groups,  $^1\text{H}$  spin-lattice relaxation dispersion profiles of proteins are described in terms of a sum of homonuclear  $^1\text{H}$ - $^1\text{H}$  and heteronuclear  $^1\text{H}$ - $^{14}\text{N}$  contributions. Standard quantitative analysis relies on formulae including power-laws or Cole-Davidson spectral density functions for the homonuclear contribution and Lorentzian or Gaussian functions for the heteronuclear counterpart [1,2]. In the present studies we make an attempt to describe the relaxation dispersion profiles of proteins by employing: 1) multi rotational-like dynamics for  $^1\text{H}$ - $^1\text{H}$  interactions and 2) quadrupolar relaxation enhancement of  $^1\text{H}$  relaxation originating from  $^1\text{H}$ - $^{14}\text{N}$  dipole-dipole interactions [3, 4].

Thorough quantitative analysis of relaxation data obtained for solid proteins: elastin, lysozyme and albumin shows, that the homonuclear contribution to the NMRD profile can be described in terms of three rotational-like dynamical processes occurring on a different time scales, ranging from  $\mu\text{s}$  to ns, and frequency independent term A. Despite structural differences between the investigated systems, the parameters characterising  $^1\text{H}$ - $^1\text{H}$  dipolar interactions (coupling constants and correlation times),  $^1\text{H}$ - $^{14}\text{N}$  couplings ( $^1\text{H}$ - $^{14}\text{N}$  distances and  $^1\text{H}$ - $^{14}\text{N}$  bond orientations) and  $^{14}\text{N}$  quadrupolar interactions (coupling constants, asymmetry parameters) are similar.

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